Filippo De Angelis

List of Publications by Year
in descending order

386 papers	42,494 citations	2322 98 h-index	2571 195 g-index
389 all docs	389 docs citations	389 times ranked	29337 citing authors

#	Article	IF	Citations
1	Combined Experimental and DFT-TDDFT Computational Study of Photoelectrochemical Cell Ruthenium Sensitizers. Journal of the American Chemical Society, 2005, 127, 16835-16847.	13.7	2,645
2	Intrinsic Thermal Instability of Methylammonium Lead Trihalide Perovskite. Advanced Energy Materials, 2015, 5, 1500477.	19.5	1,788
3	Defect migration in methylammonium lead iodide and its role in perovskite solar cell operation. Energy and Environmental Science, 2015, 8, 2118-2127.	30.8	1,278
4	Relativistic GW calculations on CH3NH3PbI3 and CH3NH3SnI3 Perovskites for Solar Cell Applications. Scientific Reports, 2014, 4, 4467.	3.3	1,093
5	Cation-Induced Band-Gap Tuning in Organohalide Perovskites: Interplay of Spinâ€“Orbit Coupling and Octahedra Tilting. Nano Letters, 2014, 14, 3608-3616.	9.1	1,033
6	First-Principles Modeling of Mixed Halide Organometal Perovskites for Photovoltaic Applications. Journal of Physical Chemistry C, 2013, 117, 13902-13913.	3.1	861
7	A molecularly engineered hole-transporting material for efficient perovskite solar cells. Nature Energy, 2016, 1, .	39.5	816
8	Molecular Engineering of Organic Sensitizers for Solar Cell Applications. Journal of the American Chemical Society, 2006, 128, 16701-16707.	13.7	760
9	Solution Synthesis Approach to Colloidal Cesium Lead Halide Perovskite Nanoplatelets with Monolayer-Level Thickness Control. Journal of the American Chemical Society, 2016, 138, 1010-1016.	13.7	747
10	MAPbI_{3-x}Cl_{<i>x</i>} Mixed Halide Perovskite for Hybrid Solar Cells: The Role of Chloride as Dopant on the Transport and Structural Properties. Chemistry of Materials, 2013, 25, 4613-4618.	6.7	732
11	Stabilizing halide perovskite surfaces for solar cell operation with wide-bandgap lead oxysalts. Science, 2019, 365, 473-478.	12.6	723
12	Titanium Dioxide Nanomaterials for Photovoltaic Applications. Chemical Reviews, 2014, 114, 10095-10130.	47.7	669
13	Molecular Engineering of Organic Sensitizers for Dye-Sensitized Solar Cell Applications. Journal of the American Chemical Society, 2008, 130, 6259-6266.	13.7	625
14	The Raman Spectrum of the CH₃NH₃PbI₃ Hybrid Perovskite: Interplay of Theory and Experiment. Journal of Physical Chemistry Letters, 2014, 5, 279-284.	4.6	555
15	Origin of the Thermal Instability in CH₃NH₃PbI₃ Thin Films Deposited on ZnO. Chemistry of Materials, 2015, 27, 4229-4236.	6.7	548
16	Migration of cations induces reversible performance losses over day/night cycling in perovskite solar cells. Energy and Environmental Science, 2017, 10, 604-613.	30.8	525
17	Large polarons in lead halide perovskites. Science Advances, 2017, 3, e1701217.	10.3	515
18	Efficient Far Red Sensitization of Nanocrystalline TiO₂ Films by an Unsymmetrical Squaraine Dye. Journal of the American Chemical Society, 2007, 129, 10320-10321.	13.7	497

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19	Nearly Monodisperse Insulator Cs₄PbX₆ (X = Cl, Br, I) Nanocrystals, Their Mixed Halide Compositions, and Their Transformation into CsPbX₃ Nanocrystals. Nano Letters, 2017, 17, 1924-1930.	9.1	488
20	Iodine chemistry determines the defect tolerance of lead-halide perovskites. Energy and Environmental Science, 2018, 11, 702-713.	30.8	480
21	Ligand-engineered bandgap stability in mixed-halide perovskite LEDs. Nature, 2021, 591, 72-77.	27.8	471
22	Defect-Assisted Photoinduced Halide Segregation in Mixed-Halide Perovskite Thin Films. ACS Energy Letters, 2017, 2, 1416-1424.	17.4	437
23	Structural and optical properties of methylammonium lead iodide across the tetragonal to cubic phase transition: implications for perovskite solar cells. Energy and Environmental Science, 2016, 9, 155-163.	30.8	423
24	<i>Ab Initio</i> Molecular Dynamics Simulations of Methylammonium Lead Iodide Perovskite Degradation by Water. Chemistry of Materials, 2015, 27, 4885-4892.	6.7	414
25	Theoretical Studies on Anatase and Less Common TiO₂ Phases: Bulk, Surfaces, and Nanomaterials. Chemical Reviews, 2014, 114, 9708-9753.	47.7	367
26	Influence of the Sensitizer Adsorption Mode on the Open-Circuit Potential of Dye-Sensitized Solar Cells. Nano Letters, 2007, 7, 3189-3195.	9.1	340
27	Broadband Emission in Two-Dimensional Hybrid Perovskites: The Role of Structural Deformation. Journal of the American Chemical Society, 2017, 139, 39-42.	13.7	336
28	A Computational Investigation of Organic Dyes for Dye-Sensitized Solar Cells: Benchmark, Strategies, and Open Issues. Journal of Physical Chemistry C, 2010, 114, 7205-7212.	3.1	328
29	Fluorescent Alloy CsPb_{<i>x</i>}Mn_{1â€“<i>x</i>}I₃ Perovskite Nanocrystals with High Structural and Optical Stability. ACS Energy Letters, 2017, 2, 2183-2186.	17.4	305
30	Light-induced annihilation of Frenkel defects in organo-lead halide perovskites. Energy and Environmental Science, 2016, 9, 3180-3187.	30.8	302
31	Extremely Slow Photoconductivity Response of CH₃NH₃PbI₃ Perovskites Suggesting Structural Changes under Working Conditions. Journal of Physical Chemistry Letters, 2014, 5, 2662-2669.	4.6	301
32	Absorption Spectrum and Solvatochromism of the [Ru(4,4â€˜-COOH-2,2â€˜-bpy)2(NCS)2] Molecular Dye by Time Dependent Density Functional Theory. Journal of the American Chemical Society, 2003, 125, 4381-4387.	13.7	299
33	Interplay of Orientational Order and Electronic Structure in Methylammonium Lead Iodide: Implications for Solar Cell Operation. Chemistry of Materials, 2014, 26, 6557-6569.	6.7	286
34	Dynamical Origin of the Rashba Effect in Organohalide Lead Perovskites: A Key to Suppressed Carrier Recombination in Perovskite Solar Cells?. Journal of Physical Chemistry Letters, 2016, 7, 1638-1645.	4.6	278
35	Controlling competing photochemical reactions stabilizes perovskite solar cells. Nature Photonics, 2019, 13, 532-539.	31.4	273
36	Alignment of the dyeâ€™s molecular levels with the TiO₂band edges in dye-sensitized solar cells: a DFTâ€“TDDFT study. Nanotechnology, 2008, 19, 424002.	2.6	263

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37	Aggregation of Organic Dyes on TiO₂ in Dye-Sensitized Solar Cells Models: An <i>ab Initio</i> Investigation. ACS Nano, 2010, 4, 556-562.	14.6	249
38	Influence of the dye molecular structure on the TiO₂conduction band in dye-sensitized solar cells: disentangling charge transfer and electrostatic effects. Energy and Environmental Science, 2013, 6, 183-193.	30.8	247
39	First-Principles Investigation of the TiO₂/Organohalide Perovskites Interface: The Role of Interfacial Chlorine. Journal of Physical Chemistry Letters, 2014, 5, 2619-2625.	4.6	247
40	The Impact of the Crystallization Processes on the Structural and Optical Properties of Hybrid Perovskite Films for Photovoltaics. Journal of Physical Chemistry Letters, 2014, 5, 3836-3842.	4.6	238
41	Controlling Phosphorescence Color and Quantum Yields in Cationic Iridium Complexes:Â A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2007, 46, 5989-6001.	4.0	237
42	Time-Dependent DFT Study of [Fe(CN)6]4-Sensitization of TiO2Nanoparticles. Journal of the American Chemical Society, 2004, 126, 15024-15025.	13.7	228
43	Time-Dependent Density Functional Theory Investigations on the Excited States of Ru(II)-Dye-Sensitized TiO₂ Nanoparticles:â€‰ The Role of Sensitizer Protonation. Journal of the American Chemical Society, 2007, 129, 14156-14157.	13.7	228
44	High Open-Circuit Voltage Solid-State Dye-Sensitized Solar Cells with Organic Dye. Nano Letters, 2009, 9, 2487-2492.	9.1	228
45	First-Principles Modeling of the Adsorption Geometry and Electronic Structure of Ru(II) Dyes on Extended TiO₂ Substrates for Dye-Sensitized Solar Cell Applications. Journal of Physical Chemistry C, 2010, 114, 6054-6061.	3.1	224
46	Synthesis, Characterization, and DFT/TD-DFT Calculations of Highly Phosphorescent Blue Light-Emitting Anionic Iridium Complexes. Inorganic Chemistry, 2008, 47, 980-989.	4.0	222
47	Absorption Spectra and Excited State Energy Levels of the N719 Dye on TiO₂ in Dye-Sensitized Solar Cell Models. Journal of Physical Chemistry C, 2011, 115, 8825-8831.	3.1	222
48	Formation of Surface Defects Dominates Ion Migration in Lead-Halide Perovskites. ACS Energy Letters, 2019, 4, 779-785.	17.4	219
49	Electronic Transitions Involved in the Absorption Spectrum and Dual Luminescence of Tetranuclear Cubane [Cu4I4(pyridine)4] Cluster:Â a Density Functional Theory/Time-Dependent Density Functional Theory Investigation. Inorganic Chemistry, 2006, 45, 10576-10584.	4.0	218
50	Structural and electronic properties of organo-halide lead perovskites: a combined IR-spectroscopy and ab initio molecular dynamics investigation. Physical Chemistry Chemical Physics, 2014, 16, 16137-16144.	2.8	211
51	Cobalt Electrolyte/Dye Interactions in Dye-Sensitized Solar Cells: A Combined Computational and Experimental Study. Journal of the American Chemical Society, 2012, 134, 19438-19453.	13.7	204
52	First-Principles Modeling of Defects in Lead Halide Perovskites: Best Practices and Open Issues. ACS Energy Letters, 2018, 3, 2206-2222.	17.4	202
53	Stark Effect in Perovskite/TiO₂ Solar Cells: Evidence of Local Interfacial Order. Nano Letters, 2014, 14, 2168-2174.	9.1	200
54	CH₃NH₃PbI₃ perovskite single crystals: surface photophysics and their interaction with the environment. Chemical Science, 2015, 6, 7305-7310.	7.4	192

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55	Defect Activity in Lead Halide Perovskites. Advanced Materials, 2019, 31, e1901183.	21.0	191
56	Photoinduced Reversible Structural Transformations in Free-Standing CH₃NH₃PbI₃ Perovskite Films. Journal of Physical Chemistry Letters, 2015, 6, 2332-2338.	4.6	190
57	Di-branched di-anchoring organic dyes for dye-sensitized solar cells. Energy and Environmental Science, 2009, 2, 1094.	30.8	188
58	Computational modelling of TiO₂surfaces sensitized by organic dyes with different anchoring groups: adsorption modes, electronic structure and implication for electron injection/recombination. Physical Chemistry Chemical Physics, 2012, 14, 920-928.	2.8	185
59	Ferroelectric Polarization of CH₃NH₃PbI₃: A Detailed Study Based on Density Functional Theory and Symmetry Mode Analysis. Journal of Physical Chemistry Letters, 2015, 6, 2223-2231.	4.6	179
60	Intrinsic Halide Segregation at Nanometer Scale Determines the High Efficiency of Mixed Cation/Mixed Halide Perovskite Solar Cells. Journal of the American Chemical Society, 2016, 138, 15821-15824.	13.7	179
61	Mobile Ions in Organohalide Perovskites: Interplay of Electronic Structure and Dynamics. ACS Energy Letters, 2016, 1, 182-188.	17.4	179
62	Elusive Presence of Chloride in Mixed Halide Perovskite Solar Cells. Journal of Physical Chemistry Letters, 2014, 5, 3532-3538.	4.6	175
63	Electronic and optical properties of mixed Snâ€“Pb organohalide perovskites: a first principles investigation. Journal of Materials Chemistry A, 2015, 3, 9208-9215.	10.3	170
64	Synthesis, Characterization, and DFT-TDDFT Computational Study of a Ruthenium Complex Containing a Functionalized Tetradentate Ligand. Inorganic Chemistry, 2006, 45, 4642-4653.	4.0	167
65	The Role of Substituents on Functionalized 1,10-Phenanthroline in Controlling the Emission Properties of Cationic Iridium(III) Complexes of Interest for Electroluminescent Devices. Inorganic Chemistry, 2007, 46, 8533-8547.	4.0	164
66	A computational approach to the electronic and optical properties of Ru(II) and Ir(III) polypyridyl complexes: Applications to DSC, OLED and NLO. Coordination Chemistry Reviews, 2011, 255, 2704-2726.	18.8	161
67	Organic dyes incorporating low-band-gap chromophores based on Ï€-extended benzothiadiazole for dye-sensitized solar cells. Dyes and Pigments, 2011, 91, 192-198.	3.7	160
68	Adsorption of organic dyes on TiO2 surfaces in dye-sensitized solar cells: interplay of theory and experiment. Physical Chemistry Chemical Physics, 2012, 14, 15963.	2.8	151
69	Influence of Surface Termination on the Energy Level Alignment at the CH₃NH₃PbI₃ Perovskite/C60 Interface. Chemistry of Materials, 2017, 29, 958-968.	6.7	149
70	Calculation of near-edge x-ray-absorption fine structure at finite temperatures: Spectral signatures of hydrogen bond breaking in liquid water. Journal of Chemical Physics, 2004, 120, 8632-8637.	3.0	148
71	Ionotronic Halide Perovskite Driftâ€Diffusive Synapses for Lowâ€Power Neuromorphic Computation. Advanced Materials, 2018, 30, e1805454.	21.0	146
72	Electronic and Optical Properties of the Spiro-MeOTAD Hole Conductor in Its Neutral and Oxidized Forms: A DFT/TDDFT Investigation. Journal of Physical Chemistry C, 2011, 115, 23126-23133.	3.1	145

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73	Instability of Tin Iodide Perovskites: Bulk p-Doping versus Surface Tin Oxidation. ACS Energy Letters, 2020, 5, 2787-2795.	17.4	143
74	Energy levels, charge injection, charge recombination and dye regeneration dynamics for donorâ€“acceptor Ï€-conjugated organic dyes in mesoscopic TiO2 sensitized solar cells. Energy and Environmental Science, 2011, 4, 1820.	30.8	140
75	Joint electrical, photophysical and computational studies on D-Ï€-A dye sensitized solar cells: the impacts of dithiophene rigidification. Chemical Science, 2012, 3, 976.	7.4	140
76	Electronic and optical properties of MAPbX₃ perovskites (X = I, Br, Cl): a unified DFT and GW theoretical analysis. Physical Chemistry Chemical Physics, 2016, 18, 27158-27164.	2.8	140
77	Modeling Excited States and Alignment of Energy Levels in Dye-Sensitized Solar Cells: Successes, Failures, and Challenges. Journal of Physical Chemistry C, 2013, 117, 3685-3700.	3.1	137
78	Large electrostrictive response in lead halide perovskites. Nature Materials, 2018, 17, 1020-1026.	27.5	137
79	Ab Initio Determination of Ground and Excited State Oxidation Potentials of Organic Chromophores for Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2010, 114, 22742-22750.	3.1	135
80	The Doping Mechanism of Halide Perovskite Unveiled by Alkaline Earth Metals. Journal of the American Chemical Society, 2020, 142, 2364-2374.	13.7	132
81	Tin versus Lead Redox Chemistry Modulates Charge Trapping and Self-Doping in Tin/Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 3546-3556.	4.6	132
82	Structural and electronic properties of organo-halide hybrid perovskites from ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2015, 17, 9394-9409.	2.8	130
83	Coumarin dyes containing low-band-gap chromophores for dye-sensitised solar cells. Dyes and Pigments, 2011, 90, 304-310.	3.7	126
84	Tuning halide perovskite energy levels. Energy and Environmental Science, 2021, 14, 1429-1438.	30.8	124
85	Time-dependent density functional theory study of the absorption spectrum of [Ru(4,4â€²-COOH-2,2â€²-bpy)2(NCS)2] in water solution: influence of the pH. Chemical Physics Letters, 2004, 389, 204-208.	2.6	121
86	Defect activity in metal halide perovskites with wide and narrow bandgap. Nature Reviews Materials, 2021, 6, 986-1002.	48.7	121
87	Single-crystalline TiO2 nanoparticles for stable and efficient perovskite modules. Nature Nanotechnology, 2022, 17, 598-605.	31.5	121
88	Direct vs. indirect injection mechanisms in perylene dye-sensitized solar cells: A DFT/TDDFT investigation. Chemical Physics Letters, 2010, 493, 323-327.	2.6	118
89	Modeling Materials and Processes in Hybrid/Organic Photovoltaics: From Dye-Sensitized to Perovskite Solar Cells. Accounts of Chemical Research, 2014, 47, 3349-3360.	15.6	117
90	Origin of low electronâ€“hole recombination rate in metal halide perovskites. Energy and Environmental Science, 2018, 11, 101-105.	30.8	113

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91	Photophysical Properties of [Ru(phen)2(dppz)]2+Intercalated into DNA:Â An Integrated Carâˆ’Parrinello and TDDFT Study. Journal of the American Chemical Society, 2005, 127, 14144-14145.	13.7	112
92	Electronic Structure and Reactivity of Isomeric Oxo-Mn(V) Porphyrins:Â Effects of Spin-State Crossing and pKaModulation. Inorganic Chemistry, 2006, 45, 4268-4276.	4.0	107
93	Electron-rich heteroaromatic conjugated bipyridine based ruthenium sensitizer for efficient dye-sensitized solar cells. Chemical Communications, 2008, , 5318.	4.1	107
94	Solvent Effects on the UV (nâ†’ Ï€*) and NMR (13C and17O) Spectra of Acetone in Aqueous Solution. An Integrated Carâˆ’Parrinello and DFT/PCM Approach. Journal of Physical Chemistry B, 2005, 109, 445-453.	2.6	106
95	High Open-Circuit Voltage: Fabrication of Formamidinium Lead Bromide Perovskite Solar Cells Using Fluoreneâ€“Dithiophene Derivatives as Hole-Transporting Materials. ACS Energy Letters, 2016, 1, 107-112.	17.4	105
96	Electrochemical Hole Injection Selectively Expels Iodide from Mixed Halide Perovskite Films. Journal of the American Chemical Society, 2019, 141, 10812-10820.	13.7	104
97	Novel Carbazole-Phenothiazine Dyads for Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study. ACS Applied Materials & Interfaces, 2013, 5, 9635-9647.	8.0	102
98	Rashba Band Splitting in Organohalide Lead Perovskites: Bulk and Surface Effects. Journal of Physical Chemistry Letters, 2017, 8, 2247-2252.	4.6	101
99	Mechanism of Reversible Trap Passivation by Molecular Oxygen in Lead-Halide Perovskites. ACS Energy Letters, 2017, 2, 2794-2798.	17.4	100
100	Simulating Dye-Sensitized TiO₂ Heterointerfaces in Explicit Solvent: Absorption Spectra, Energy Levels, and Dye Desorption. Journal of Physical Chemistry Letters, 2011, 2, 813-817.	4.6	98
101	Cyclometalated Iridium(III) Complexes Based on Phenyl-Imidazole Ligand. Inorganic Chemistry, 2011, 50, 451-462.	4.0	98
102	Ultrafast THz Probe of Photoinduced Polarons in Lead-Halide Perovskites. Physical Review Letters, 2019, 122, 166601.	7.8	98
103	Tuning structural isomers of phenylenediammonium to afford efficient and stable perovskite solar cells and modules. Nature Communications, 2021, 12, 6394.	12.8	98
104	Understanding Performance Limiting Interfacial Recombination in <i>pin</i> Perovskite Solar Cells. Advanced Energy Materials, 2022, 12, .	19.5	95
105	White-light phosphorescence emission from a single molecule: application to OLED. Chemical Communications, 2009, , 4672.	4.1	92
106	Time dependent density functional theory study of the absorption spectrum of the [Ru(4,4â€²-COOâˆ’-2,2â€²-bpy)2(X)2]4âˆ’ (X=NCS, Cl) dyes in water solution. Chemical Physics Letters, 2005, 415, 115-120.	2.6	91
107	Multication perovskite 2D/3D interfaces form via progressive dimensional reduction. Nature Communications, 2021, 12, 3472.	12.8	89
108	Infrared Dielectric Screening Determines the Low Exciton Binding Energy of Metal-Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 620-627.	4.6	88

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109	Modeling the Interaction of Molecular Iodine with MAPbI₃: A Probe of Lead-Halide Perovskites Defect Chemistry. ACS Energy Letters, 2018, 3, 447-451.	17.4	88
110	Cyclometallated iridium(iii) complexes with substituted 1,10-phenanthrolines: a new class of highly active organometallic second order NLO-phores with excellent transparency with respect to second harmonic emission. Chemical Communications, 2007, , 4116.	4.1	87
111	Computational Investigation of Dyeâ€"Iodine Interactions in Organic Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2012, 116, 5965-5973.	3.1	86
112	A TDDFT study of the ruthenium(II) polyazaaromatic complex [Ru(dppz)(phen)2]2+ in solution. Chemical Physics Letters, 2004, 396, 43-48.	2.6	84
113	Polarons in Metal Halide Perovskites. Advanced Energy Materials, 2020, 10, 1902748.	19.5	84
114	Solvent Effects on the Adsorption Geometry and Electronic Structure of Dye-Sensitized TiO₂: A First-Principles Investigation. Journal of Physical Chemistry C, 2012, 116, 5932-5940.	3.1	83
115	Terpyridine Zn(II), Ru(III), and Ir(III) Complexes:â€‰ The Relevant Role of the Nature of the Metal Ion and of the Ancillary Ligands on the Second-Order Nonlinear Response of Terpyridines Carrying Electron Donor or Electron Acceptor Groups. Inorganic Chemistry, 2005, 44, 8967-8978.	4.0	82
116	Time-dependent density functional theory study of squaraine dye-sensitized solar cells. Chemical Physics Letters, 2009, 475, 49-53.	2.6	82
117	Supramolecular Interactions of Chenodeoxycholic Acid Increase the Efficiency of Dye-Sensitized Solar Cells Based on a Cobalt Electrolyte. Journal of Physical Chemistry C, 2013, 117, 3874-3887.	3.1	82
118	Universal approach toward high-efficiency two-dimensional perovskite solar cells <i>via</i> a vertical-rotation process. Energy and Environmental Science, 2020, 13, 3093-3101.	30.8	82
119	Globularityâ€Selected Large Molecules for a New Generation of Multication Perovskites. Advanced Materials, 2017, 29, 1702005.	21.0	81
120	Ligand Engineering for the Efficient Dye-Sensitized Solar Cells with Ruthenium Sensitizers and Cobalt Electrolytes. Inorganic Chemistry, 2016, 55, 6653-6659.	4.0	80
121	A Combined Computational and Experimental Study of Polynuclear Ruâ^'TPPZ Complexes:Â Insight into the Electronic and Optical Properties of Coordination Polymers. Journal of the American Chemical Society, 2004, 126, 9715-9723.	13.7	78
122	Absorption and Emission of the Apigenin and Luteolin Flavonoids: A TDDFT Investigation. Journal of Physical Chemistry A, 2009, 113, 15118-15126.	2.5	77
123	Stable Ligand Coordination at the Surface of Colloidal CsPbBr₃ Nanocrystals. Journal of Physical Chemistry Letters, 2019, 10, 3715-3726.	4.6	77
124	Intermolecular Interactions in Dye-Sensitized Solar Cells: A Computational Modeling Perspective. Journal of Physical Chemistry Letters, 2013, 4, 956-974.	4.6	76
125	Inherent electronic trap states in TiO2 nanocrystals: effect of saturation and sintering. Energy and Environmental Science, 2013, 6, 1221.	30.8	76
126	Bi-functional interfaces by poly(ionic liquid) treatment in efficient pin and nip perovskite solar cells. Energy and Environmental Science, 2021, 14, 4508-4522.	30.8	76

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127	Solvents for Processing Stable Tin Halide Perovskites. ACS Energy Letters, 2021, 6, 959-968.	17.4	76
128	Understanding the Solution Chemistry of Lead Halide Perovskites Precursors. ACS Applied Energy Materials, 2019, 2, 3400-3409.	5.1	74
129	Theoretical design of phosphorescence parameters for organic electro-luminescence devices based on iridium complexes. Chemical Physics, 2009, 358, 245-257.	1.9	73
130	Interplay of Stereoelectronic and Enviromental Effects in Tuning the Structural and Magnetic Properties of a Prototypical Spin Probe:Â Further Insights from a First Principle Dynamical Approach. Journal of the American Chemical Society, 2006, 128, 4338-4347.	13.7	72
131	From Large to Small Polarons in Lead, Tin, and Mixed Leadâ€“Tin Halide Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 1790-1798.	4.6	72
132	Waterâ€Stable DMASnBr₃ Leadâ€Free Perovskite for Effective Solarâ€Driven Photocatalysis. Angewandte Chemie - International Edition, 2021, 60, 3611-3618.	13.8	72
133	Optical Properties and Aggregation of Phenothiazine-Based Dye-Sensitizers for Solar Cells Applications: A Combined Experimental and Computational Investigation. Journal of Physical Chemistry C, 2013, 117, 9613-9622.	3.1	70
134	Influence of Donor Groups of Organic Dâˆ'Ï€â€“A Dyes on Open-Circuit Voltage in Solid-State Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2012, 116, 1572-1578.	3.1	69
135	Engineering of thiocyanate-free Ru(ii) sensitizers for high efficiency dye-sensitized solar cells. Chemical Science, 2013, 4, 2423.	7.4	67
136	Cyclometalated Ir^{III} Complexes with Substituted 1,10â€Phenanthrolines: A New Class of Efficient Cationic Organometallic Secondâ€Order NLO Chromophores. Chemistry - A European Journal, 2010, 16, 4814-4825.	3.3	65
137	Luminescent cyclometallated Ir(iii) and Pt(ii) complexes with Î²-diketonate ligands as highly active second-order NLO chromophores. Chemical Communications, 2010, 46, 2414.	4.1	64
138	Water Oxidation by the [Co4O4(OAc)4(py)4]+ Cubium is Initiated by OHâ€“ Addition. Journal of the American Chemical Society, 2015, 137, 15460-15468.	13.7	64
139	First-Principles Modeling of Bismuth Doping in the MAPbI₃ Perovskite. Journal of Physical Chemistry C, 2018, 122, 14107-14112.	3.1	64
140	Ligand-Induced Surface Charge Density Modulation Generates Local Type-II Band Alignment in Reduced-Dimensional Perovskites. Journal of the American Chemical Society, 2019, 141, 13459-13467.	13.7	62
141	Tuning the Photoinduced O2-Evolving Reactivity of Mn4O47+, Mn4O46+, and Mn4O3(OH)6+ Manganeseâˆ'Oxo Cubane Complexes. Inorganic Chemistry, 2006, 45, 189-195.	4.0	60
142	Tetraaryl Zn^{II} Porphyrinates Substituted at Î²â€Pyrrolic Positions as Sensitizers in Dyeâ€Sensitized Solar Cells: A Comparison with <i>meso</i>â€Disubstituted Pushâ€“Pull Zn^{II} Porphyrinates. Chemistry - A European Journal, 2013, 19, 10723-10740.	3.3	60
143	Enhanced TiO₂/MAPbI₃ Electronic Coupling by Interface Modification with PbI₂. Chemistry of Materials, 2016, 28, 3612-3615.	6.7	60
144	Long-Lived Photoinduced Polarons in Organohalide Perovskites. Journal of Physical Chemistry Letters, 2017, 8, 3081-3086.	4.6	59

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145	Solvent-Free Synthetic Route for Cerium(IV) Metalâ€“Organic Frameworks with UiO-66 Architecture and Their Photocatalytic Applications. ACS Applied Materials & Interfaces, 2019, 11, 45031-45037.	8.0	58
146	Panchromatic ruthenium sensitizer based on electron-rich heteroarylvinylene Ï€-conjugated quaterpyridine for dye-sensitized solar cells. Dalton Transactions, 2011, 40, 234-242.	3.3	57
147	Band Gap Engineering in MASnBr₃ and CsSnBr₃ Perovskites: Mechanistic Insights through the Application of Pressure. Journal of Physical Chemistry Letters, 2019, 10, 7398-7405.	4.6	57
148	Surface Reconstruction Engineering with Synergistic Effect of Mixedâ€Salt Passivation Treatment toward Efficient and Stable Perovskite Solar Cells. Advanced Functional Materials, 2021, 31, 2102902.	14.9	57
149	Computational Modeling of Stark Effects in Organic Dye-Sensitized TiO₂ Heterointerfaces. Journal of Physical Chemistry Letters, 2011, 2, 1261-1267.	4.6	56
150	Optical properties of ZnO nanostructures: a hybrid DFT/TDDFT investigation. Physical Chemistry Chemical Physics, 2011, 13, 467-475.	2.8	56
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